Efficient Safety and Degradation Modeling of Automotive Li-ion Cells and Pack

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EC Power

http://www.ecpowergroup.com

6/9/15

Project ID # ES200

Overview

Timeline

- Start date: 10/1/2013
- End date: 9/30/2015
- Project 75% complete

Barriers

- Barriers addressed
  - LiB Safety/Abuse
  - LiB Lifetime
  - LiB Efficiency
  - Computer tools for design exploration

Budget

- Total project funding: $2.0M
  - $1.0M (DOE)
  - $1.0M (cost share)
  - Fed. cost through 3/30/15: $380 k

Partners

- Penn State

Funding provided by **Dave Howell** of the DOE Vehicle Technologies Program .
The activity is managed by **Brian Cunningham** of Vehicle Technologies,
through NETL, **Bruce Mixer** Technical Monitor

Project Objectives - Relevance

- Develop an efficient & robust pack-level safety and abuse model
  - Predictive tool with electrochemical-thermal (ECT) coupling
  - Virtual tool to assess/screen safety of cell/pack designs
- Develop mechanism-based, fundamental models for accurately predicting degradation of Li-ion batteries
  - Predictive models valid under user-specified and wide-ranging temperatures and operating conditions
- Perform co-simulation of our software with structural mechanics software via the Open Architecture Standard (OAS)
  - Electrochemical-Thermal-Mechanical (ECT-M) coupled simulation
- Perform testing and validate the cell- and pack-level safety and degradation models
- Expand extensive materials database
  - Experimentally characterizing and adding NCA to our database
- Develop commercial software to be used by licensees
- Support DOE CAEBAT activity

Project Milestones & Activities

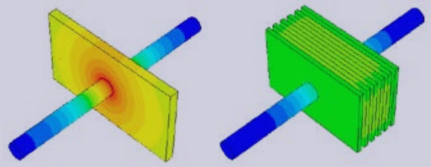
Recent Milestones Completed
M5: Materials database characterization 50% complete
M6: Initial model implementation complete for safety, abuse and degradation
M7: Budget period #1 Exit (12/31/14): Go/No-Go
M12: Complete NCA material characterization

Milestones in Progress
M8: Safety & abuse testing 100% complete (will be complete 5/1/2015)
M9: Degradation testing complete (activity delayed – see future work & summary)
M10: Complete validation of safety and abuse models (9/2015)
M11: Complete validation of degradation models (9/2015)
M13: NCA added to materials database (9/2015)
M14: Co-simulation with structural mechanics via OAS (9/2015)
M15: Final model implementation and closeout (9/2015)

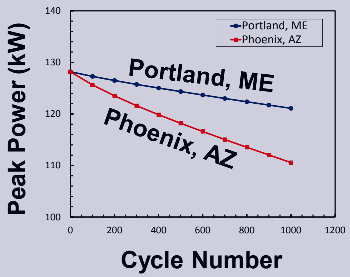
Approach – Supporting CAEBAT Activity

Modeling

Safety/Abuse

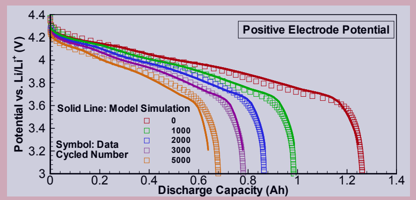


Life

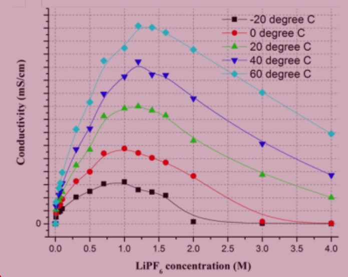


Co-Sim. via OAS (ECT-M)

Validation



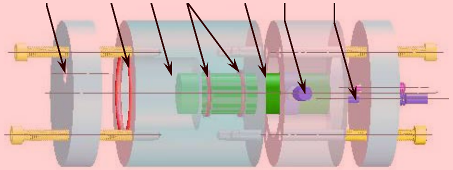
Materials Database



Experimental

Safety Testing

Life Testing

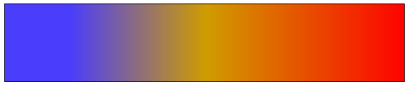


Materials Char.

*End Product: **<u>Experimentally validated</u> <u>commercial tool</u>** with advanced **<u>safety/abuse and life models</u>**, along with **<u>commercially-relevant materials database</u>***

Approach – Materials Database

Tested temperature range for materials

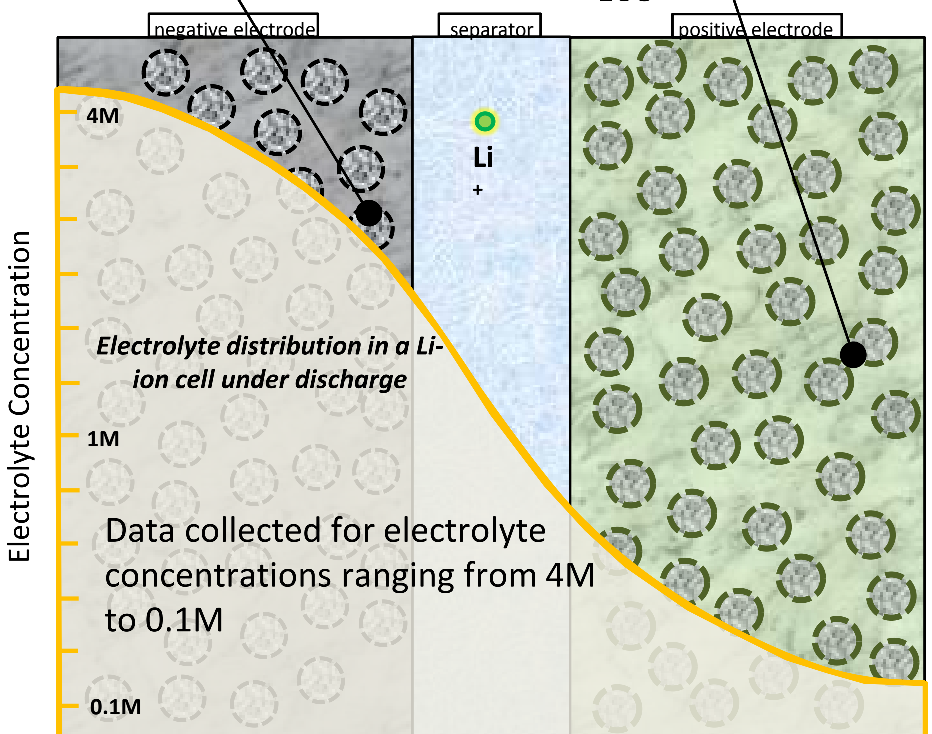
-30°C  100°C

Existing Anode Materials:

- Graphite (blend natural/syn.)
- LTO

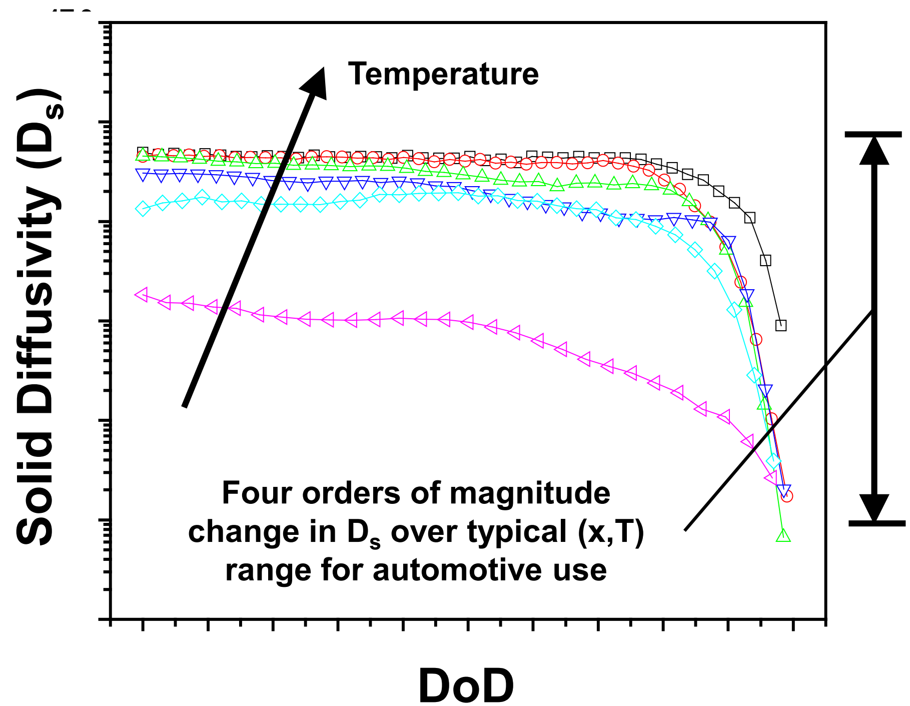
Existing Cathode materials:

- NCM
- LFP
- LMO
- LCO



Adding NCA as part of this project

- GITT for $D_s = f(T,x)$ and $OCP = f(T,x)$
- EIS for $i_o = f(T,x,c_e)$



Modeling parameters needed at ***low-T, high-T, wide range of chemical compositions*** and similar conditions of interest for ***automotive Li-ion batteries and packs***

Approach – ECT Modeling

Electrochemical Processes
- electrochemical reactions
- solid state diffusion
- ion transport through electrolyte
- charge transfer

Heat generation rate

$$q = \sum_j a_{sj} \bar{i}_{nj} \left(\bar{\eta}_j + \Pi_j \right) - \sum_k \left[< \mathbf{i}_k > \cdot \nabla < \phi_k >^k \right]$$

Thermal Processes

- conservation of thermal energy

$$\frac{\partial \left(\rho c_p T \right)}{\partial t} = \nabla \cdot \boldsymbol{\lambda} \nabla T + q$$

Temperature-dependent physico-chemical properties

$$\Phi = \Phi_{ref} \exp \left[\frac{E_{act,\Phi}}{R} \left(\frac{1}{T_{ref}} - \frac{1}{T} \right) \right]$$

Model predictions
- potential and current curves
- temperature history/distribution
- active material utilization
- current distribution

- Understanding thermal phenomena & thermal control has huge impact on
  - Battery safety
  - Cycle life
  - Battery management system
  - Cost
- Electrochemical-thermal (ECT) coupling required for
  - Safety simulations
  - Thermal runaway
  - High power, low-T operation
  - Heating from subzero environment

Accomplishments – Summary

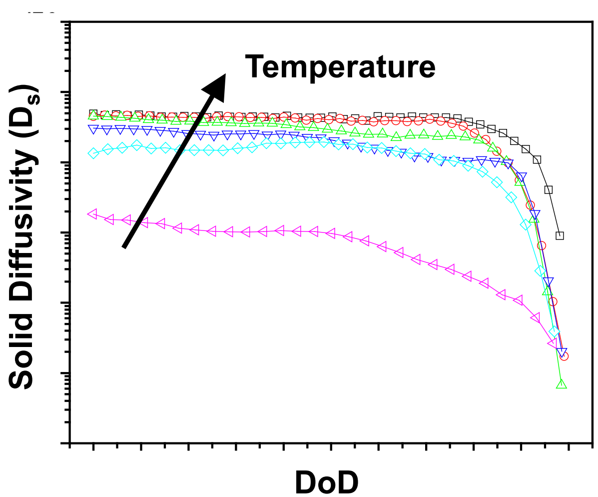
- Materials Database
  - Completed characterization over ($-40^oC < T < 60^oC$) for NCA
- Pack-level safety
  - Completed safety modeling for cells in series and parallel
  - Initial validation complete
- Abuse modeling
  - Initial overcharge models in place for NMC111 and NCA
  - Initial overcharge validation complete
  - Refinement of overcharge model and additional validation ongoing
- Life modeling
  - Electrode swelling effect added to model
  - Effect of swelling on electrode pulverization ongoing

Accomplishments – Materials Database

NCA Property Measurement

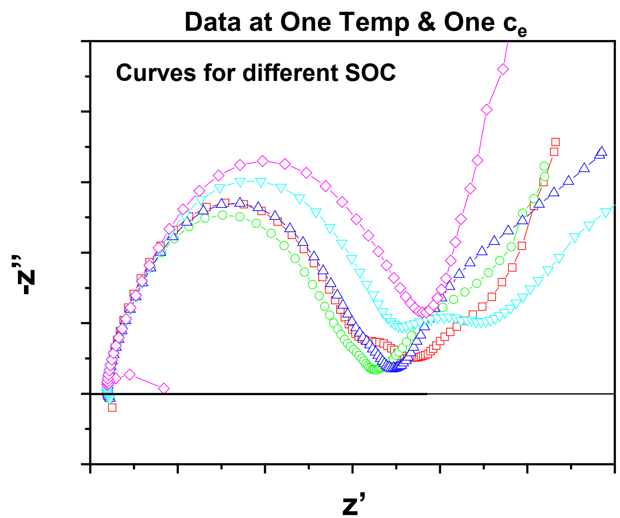
GITT Test – OCP and Ds

- Used to acquire OCP = f(x,T) and D_s = f(x,T) [x = active material stoichiometry]
- Took 8 months to carry out full matrix of (x,T) combinations
- At one T, 40+ data points to get data for entire (0 < SOC < 1) range
- NCA/Li half cells were used to acquire data



EIS – Exchange Current Density

- Used to acquire $i_o = f(x,c_e,T)$
- Took 12 months to carry out full matrix of (x,c_e,T) combinations
- NCA/Li half cells were used to acquire data
- Full range of i_o for cyclable stoich range, ($-40^oC < T < 60^oC$), and ($0.3 < c_e < 1.6M$) now complete



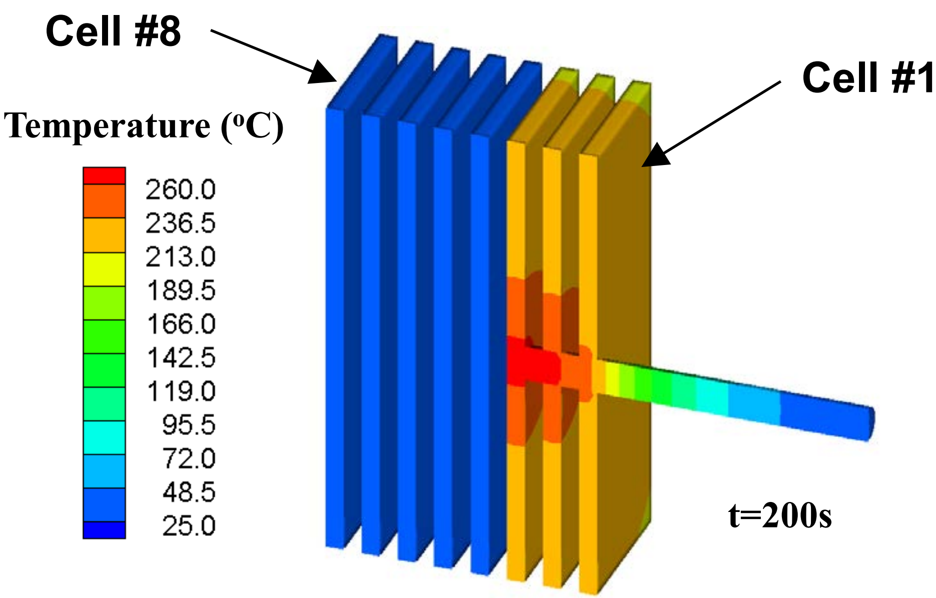
NCA characterization 100% complete

*Adding **NCA properties** to **materials database** for accurate Li-ion battery prediction under **automotive conditions***

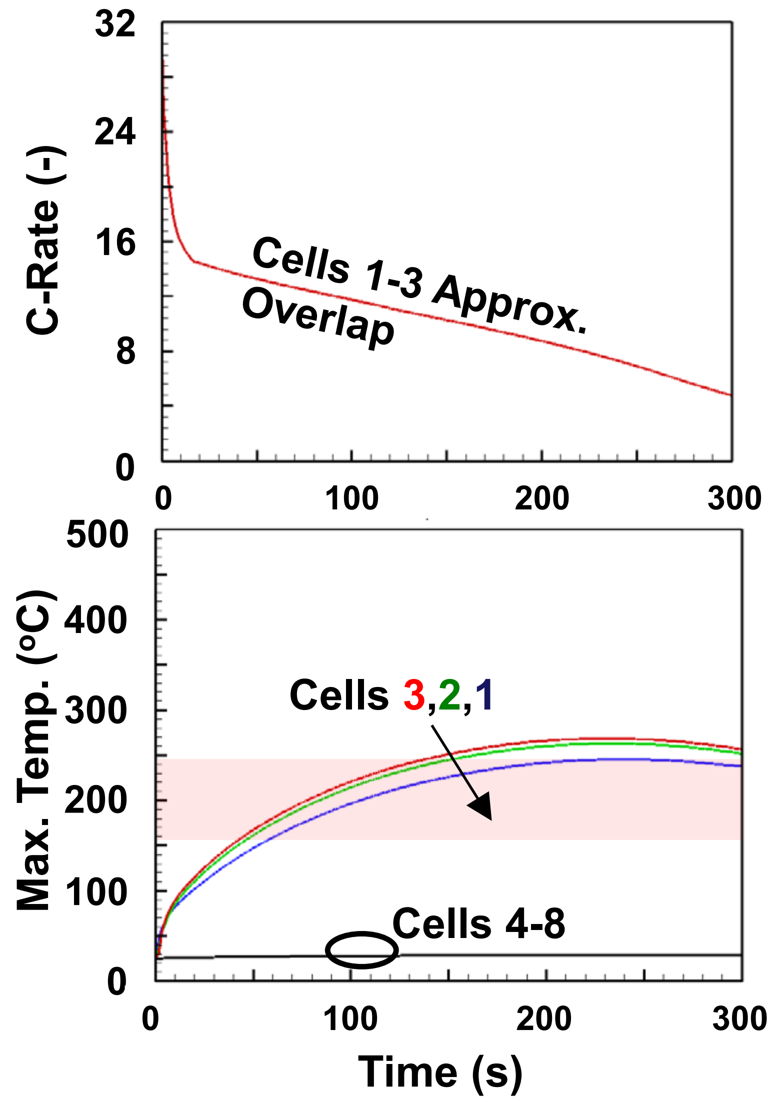
Accomplishments – Pack-level Safety

Cells in Series: 3/8 cells shorted

- 5Ah NMC111/graphite cells
- 10mm stainless steel nail used
- 3/8 ***serially*** connected cells shorted
- Unshorted cells do not discharge and remain largely cool
- Cell #3 (inner-most shorted cell) is hottest
  - Discharge of cells 1-3 approximately same rate
  - Heat rejection of cell #3 poorer than #1 & #2
- Thermal runaway likely, but after ~ 50-150s



*Tabs not shown and plot shows cutaway of center.

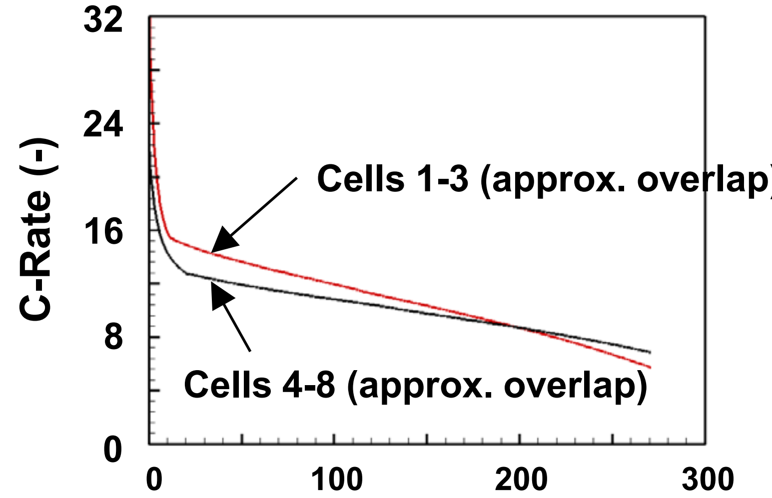


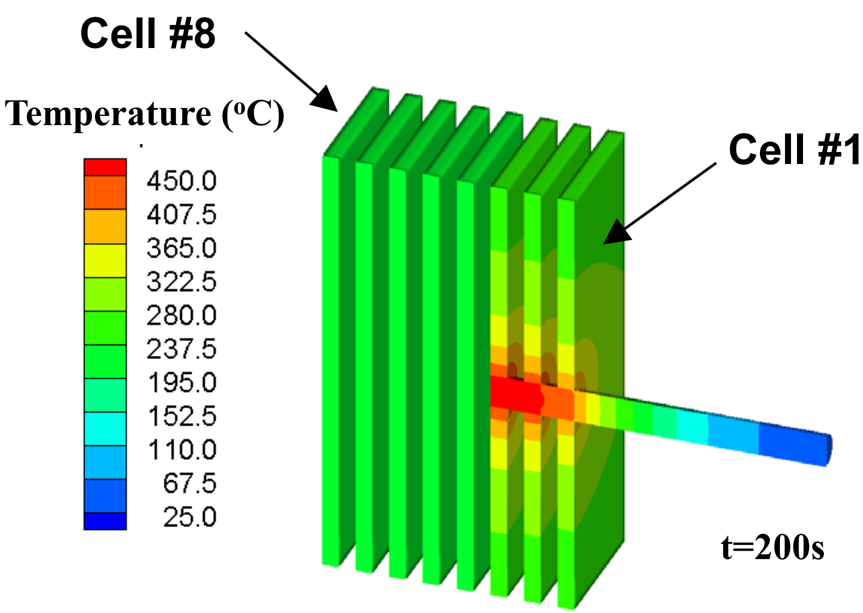
Software used to rapidly and cost effectively assess safety of cell and pack design; cell configuration considered.

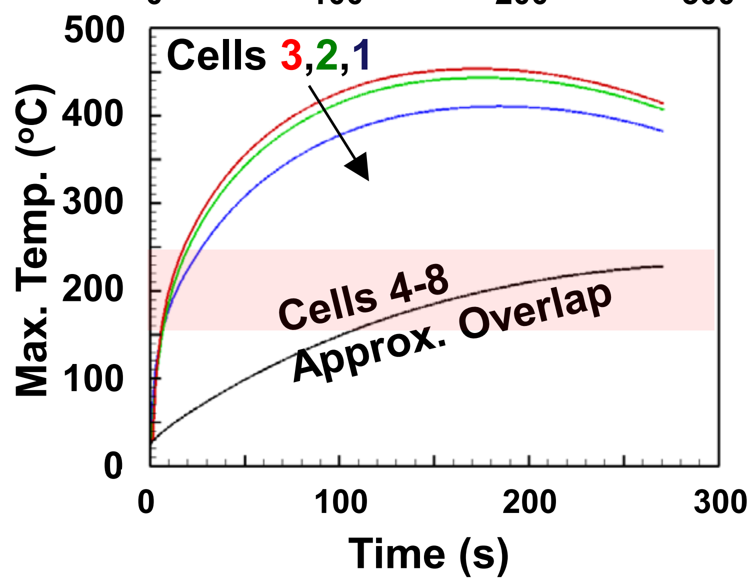
Accomplishments – Pack-level Safety

Cells in Parallel: 3/8 cells shorted

- 5Ah NMC111/graphite cells
- 10mm stainless steel nail used
- 3/8 ***parallel*** connected cells shorted
- Unshorted cells heat globally as they discharge their energy through the shorted cells/nail
- Cell #3 (inner-most shorted cell) is hottest
- Parallel connected cells much more dangerous
  - Thermal runaway conditions reached within seconds







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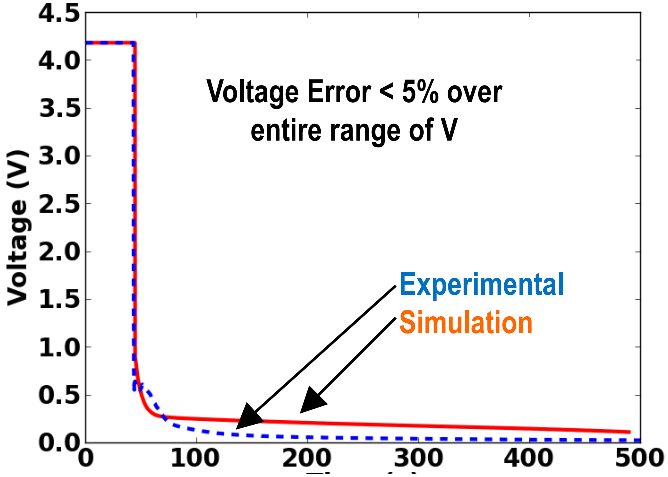
Software used to rapidly and cost effectively assess safety of cell and pack design; cell configuration considered.

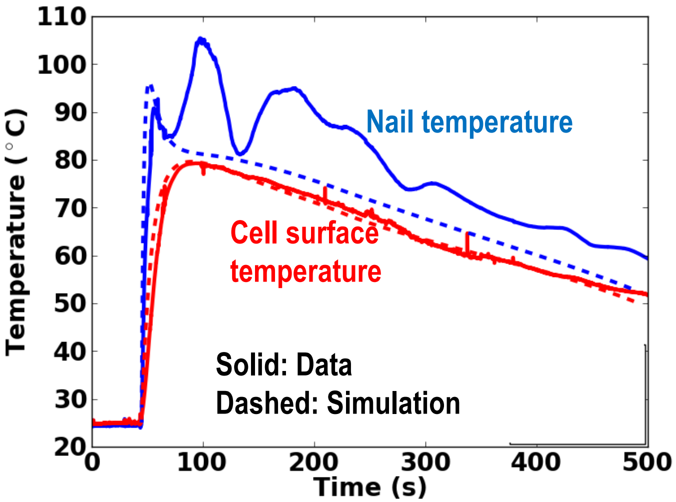
Accomplishments – Safety Validation

Preliminary Nail Penetration Validation

Validation data

- PSU has carried out one cell nail penetration test through 4/1/15: validation shown at right
- PSU will complete additional cell and module nail penetration tests for validation of software by May, 2015



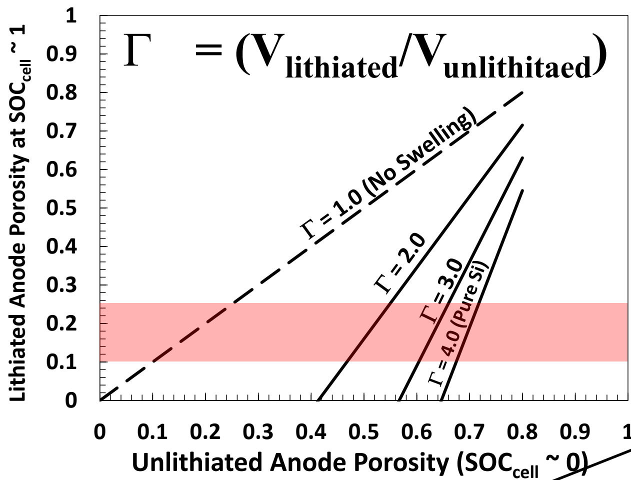


Additional nail penetration tests ongoing to assess reproducibility/quality of validation data. Physically, why is nail temp wavy after ~ 20s?

Develop and validate model of ECT response of cell/pack during nail penetration process

Accomplishments – Life & Abuse

Electrode Swelling

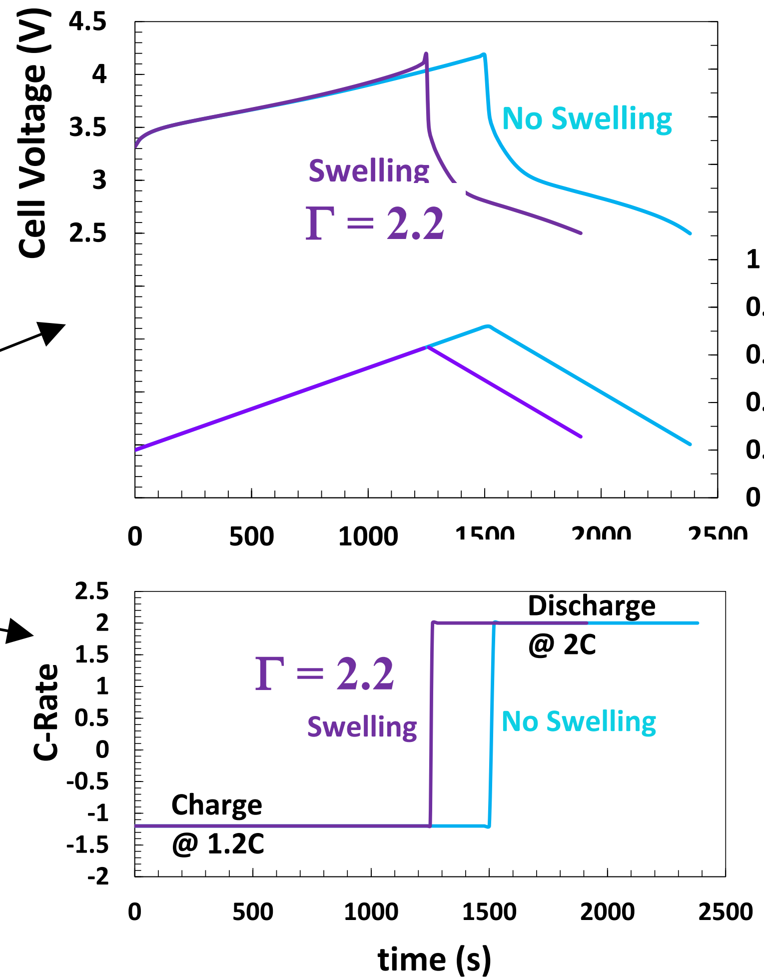


Simulation to the right:

- **Initial SOC = 0.2**
- **Fast Charge: Charge @ 1.2C until V_{cell} = 4.2V, then discharge @ 2C**

Incorporating Swelling:

- **> 10% difference in SOC that can be put into battery before upper voltage limit is reached (>10% less predicted w/swelling effects considered)**
  - **Modeling swelling of electrode critical for accurate prediction**



Active material swelling has a profound effect on performance and life.

Accomplishments – Life & Abuse

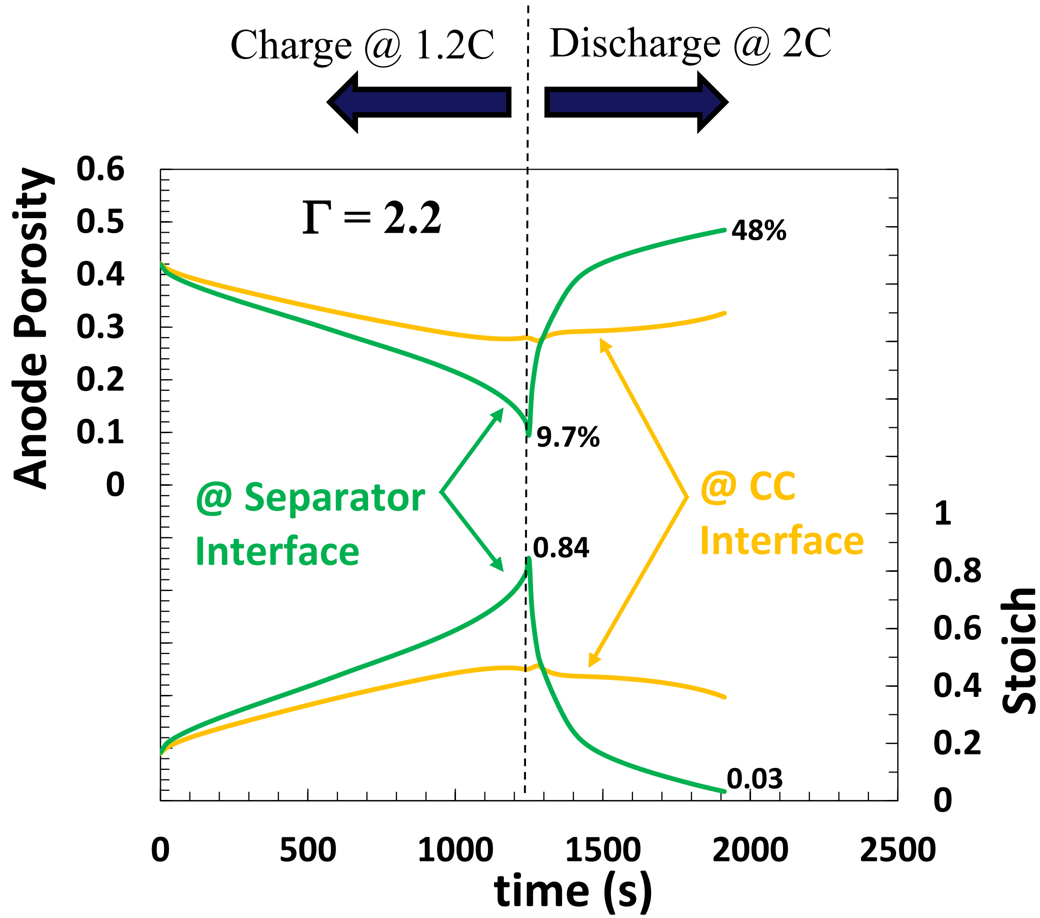
Electrode Swelling

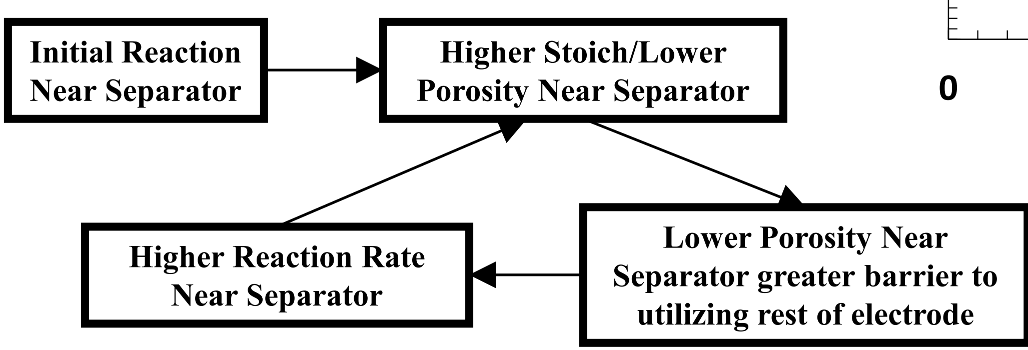
***Simulation to the right*:**

- **$SOC_o = 0.2$**
- **Fast Charge: Charge @ 1.2C until V_{cell} = 4.2V, then discharge @ 2C**

Why does swelling matter?:

- **As $SOC_{cell} \rightarrow 1$, anode stoich becomes large (~ 0.84 @ sep), porosity becomes low (< 10% @ sep), and lithiation of anode becomes difficult**
- **Anode region near separator will be utilized much more frequently and will age at a much higher rate**



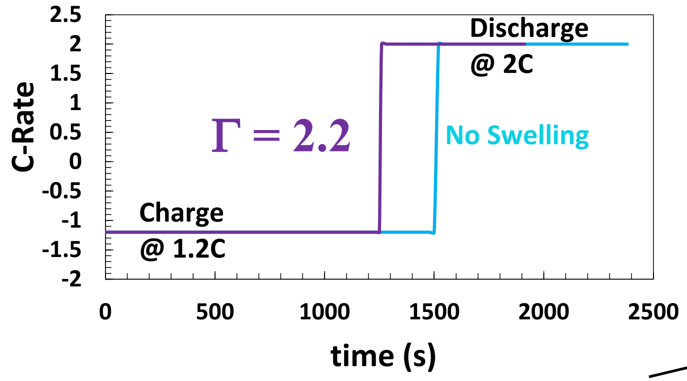


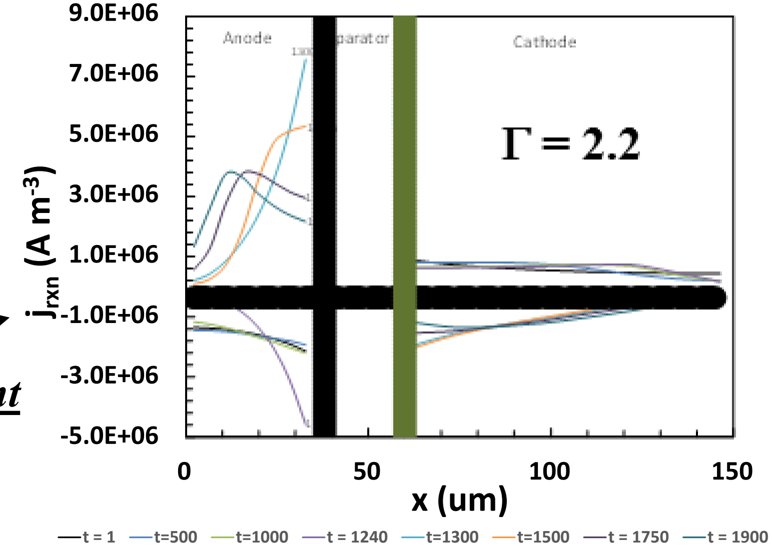
Active material swelling has a profound effect on performance and life.

Accomplishments – Life & Abuse

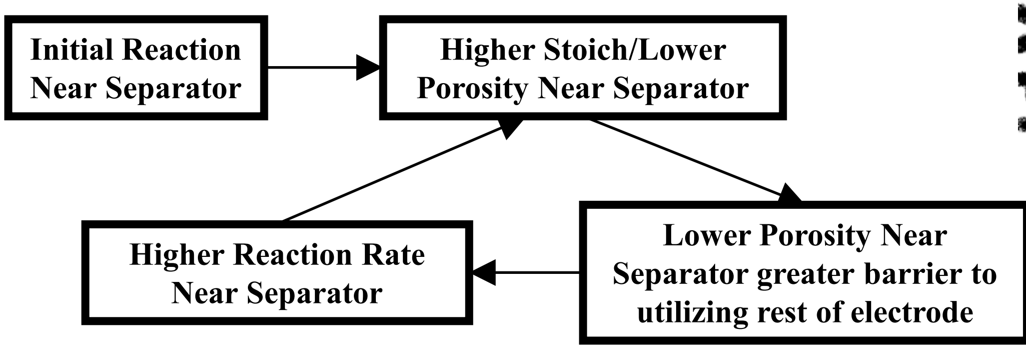
EC POWER

Electrode Swelling





- *Swelling leads to* ***highly non-uniform reaction current*** *in anode.*
- *Low porosity near separator leads to* ***poor utilization of anode active material*** *and substantially reduced cell energy density.*
- *Localized electrode pulverization most severe near separator due to greater swelling/cycling in that region*



Active Matrix

Detached Material

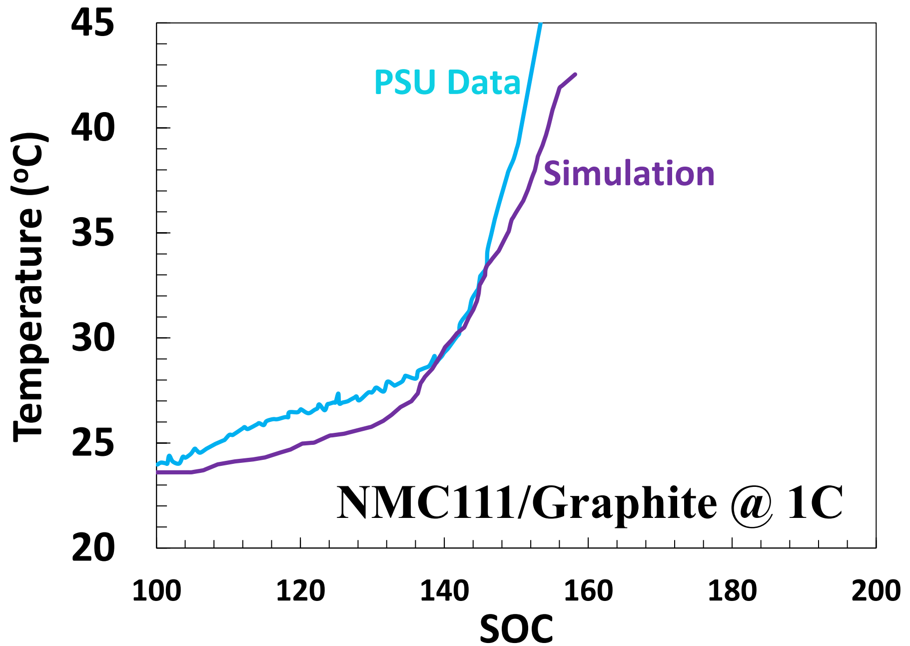
Electrode pulverization due to repeated swelling currently being completed in model

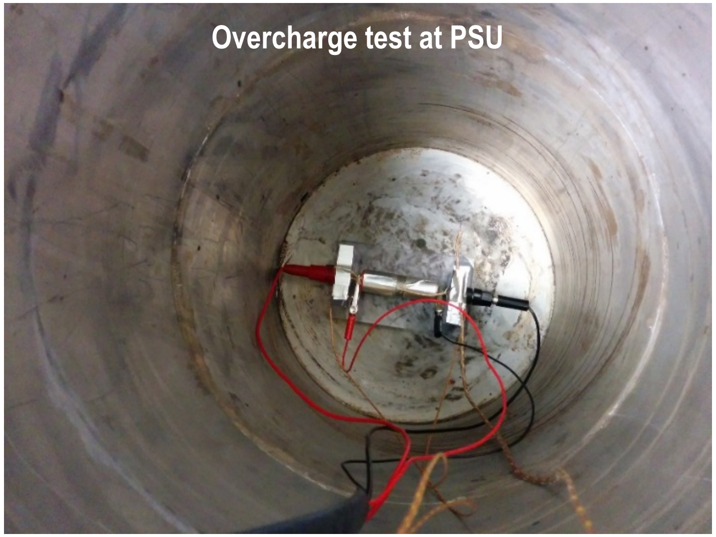
Active material swelling has a profound effect on performance and life.

Accomplishments – Life & Abuse

Overcharge modeling and validation

- PSU has carried out multiple overcharge tests for [NCA and NMC(111)], graphite 18650 cells
- EC Power has completed initial implementation of physics-based overcharge models, accounting for different C-rates, temperatures, and active materials
- Initial validation for NMC111/graphite overcharge at 1C shown below
- Model refinement and additional validation based on recently produced test data ongoing





Physics-based & validated modeling of overcharge of commercially used cells.

Collaboration w/Other Institutions

Funding Agency

Administrator

Open Architecture Software

Project Lead – Software development and sales, project administration.

Academic Partner – materials testing and detailed model validation

Future Work

- Complete nail penetration validation and model refinement
  - Single cell – validation based on additional PSU data sets
  - Multi-cell pack
- Complete implementation and validation of enhanced models for life and abuse
  - Overcharge testing – validation with NCA, different conditions, using additional test data from PSU
  - Life testing and validation – see Summary slide
- OAS: co-simulation with structural mechanics software (ECT-M simulation)
  - Plan in place – execute in 2015
- These activities reflected in future milestones

Response to Previous Year Review

- Reviewer 1: Broaden nail material and size in NP testing.
  - Within the scope of the project, we don't have resources to so this. However, we can readily simulate different nail sizes, materials (e.g. ceramic), and speeds.
- Reviewer 2: Will this modeling be readily integrated into the CAEBAT platform and the OAS developed by ORNL?
  - Yes. The final software will be compatible with OAS.
- Reviewer 3: It is not clear if the pack level shorting model will be applicable to other shorting induced incidents such as crush.
  - Through the OAS activity in this project, we aim to perform crush/internal shorting. We will use our internal shorting model to perform this task.
- Reviewer 2: It will be very useful to extend the life model to include both storage calendar life and cycle life at various temperatures.
  - Physically, our physics-based life models should accurately predict calendar life. Given the time frame, scope, and funding of the current work we do not have plans to acquire validation data for calendar life.
- Reviewer 2: What is the clear role of PSU on this work?
  - PSU leads activities related to data acquisition for abuse, life, & materials characterization.
- Reviewer 2: How much of the ECT simulation is in OAS?
  - Nothing shown thus far utilizes OAS. However, software will be compatible with OAS.

Summary

- Project on track except life testing
  - Pack-level nail penetration modeling completely implemented
  - NCA characterization complete
  - Nail penetration testing wrapping up and validation ongoing (cell and module)
  - Initial models for life and abuse have been implemented – model refinement and validation ongoing
- Life testing
  - Hurdles related to fabrication of large-format cells overcome
  - Testing to kick off May, 2015
- Future work tied to milestones and addresses project objectives
- Software is commercially available
- Meeting CAEBAT/DOE goals
  - Helping to accelerate the adoption of automotive Li-ion batteries by addressing barriers to adoption (e.g. life and safety)
  - Enabling technology for EV, PHEV